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X-Ray Resonant Raman Scattering Studies of Novel Lithium Ion Batteries

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Beamline(s): X21

Introduction: The emergence of portable telecommunication, IT and ultimately hybrid electric vehicles has created a substantial interest in manufacturing rechargeable batteries that are less expensive, non-toxic and environmentally safe, operate for longer time, are small in size and weigh less. Li-ion batteries are responding to these needs and are taking an increasing share of the rechargeable battery market. In order to improve Li-ion battery technology further, understanding the electronic structure and the redox chemistry of battery materials is of fundamental importance. The Kβ resonant Raman scattering makes it possible to study *in situ* the element specific electronic structure and follow changes in it during the battery charge-discharge cycle.

Methods and Materials: We have studied the $LiNi_{0.85}Co_{0.15}O_2$ cathode material, which was incorporated into custom made Li-ion batteries equipped with suitable x-ray windows enabling *in situ* studies of the cathode during the charge-discharge cycle. We have used Ni Kβ resonant Raman scattering technique to study the evolution of Ni electronic structure. We have measured as a function of battery charge the Kβ emission line and the Ni K-edge absorption spectrum. The absorption spectra were measured by monitoring the intensity of the Kβ emission over a narrow energy range while scanning the incident energy over the interesting absorption edge. This so-called partial yield method effectively removes the K-shell lifetime broadening and enables us to follow especially the evolution of the 1*s*→3*d* transition region with higher intrinsic resolution than in conventional absorption spectroscopy.

Results: The Kβ emission line measured at different battery charge states is shown in Fig.1. We observe changes in the emission line profile, which can be attributed to changes in the Ni valence electrons. In Fig.2. we show the evolution of the 1*s*→3*d* transition region measured using partial yield method. As we now probe directly the empty Ni 3*d* states, we observe a clear change in the spectra as the battery is charged. We have used charge-transfer multiplet calculations to quantitatively analyze the spectra.

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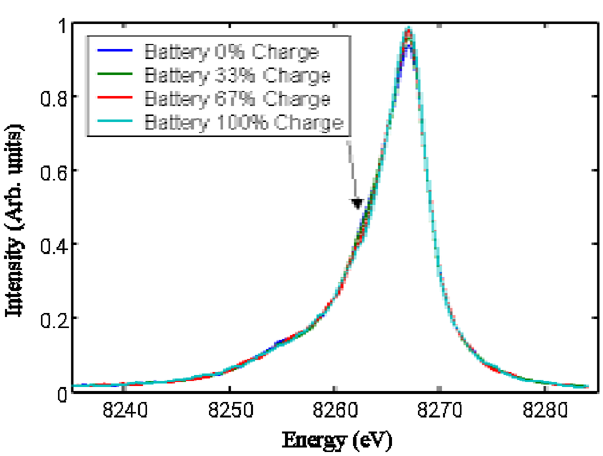

Fig. 1. The Kβ emission line measured at different battery charge states. We observe a systematic reduction of satellite intensity (arrow) as a function of battery charge.

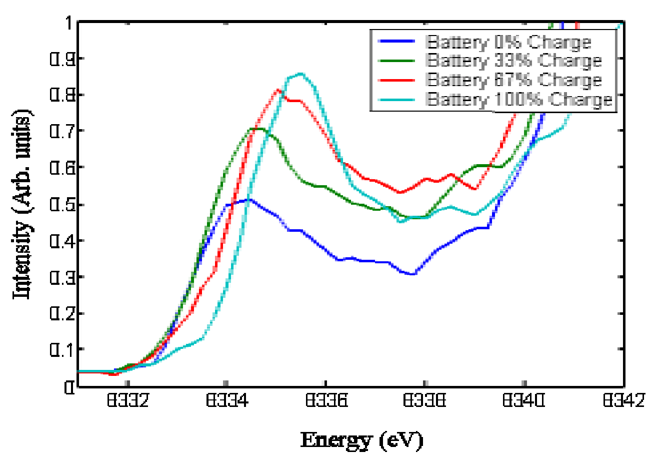

Fig. 2. The partial yield spectra of the 1*s*→3*d* transition region measured at different battery charge states. We observe a systematic change in the position and in the intensity as a function of battery charge.